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Collective water vibrations in a DNA hydration shell

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In aqueous salt solutions, DNA structure adopts a double-helical shape due to the interactions with water molecules and metal ions around the macromolecule. The ion-hydration shell stabilizes the double helix and may be considered as an integral part of the DNA structure. In the present work, the collective dynamics of DNA hydration shell is studied using classical all-atom molecular dynamics approaches. The spectra of vibrational density of states (VDOS) for water molecules around DNA double helix have been analyzed in details. The results have shown that VDOS spectra of the DNA hydration shell may be approximated by 6 vibrational modes in the range from 30 cm^{-1} to 300 cm^{-1}. The modes demonstrate significant differences in the collective vibrational dynamics of water molecules in the DNA hydration shell, compared to the bulk water. This deviation occurs due to enhanced non-bonded interactions of DNA atomic groups with water molecules constraining their mobility. In particular, our calculations have shown the complete damping of symmetrical stretching vibrations of hydrogen bonds between water molecules (the mode near 160 cm^{-1}), being present in the bulk. Such detailed atomistic analysis of water collective motions has been applied to DNA systems for the first time. This can provide a qualitative interpretation of the potential experimental data on DNA solutions. The foregoing results can shed light on fundamental processes of DNA function in a living cell, particularly, indirect protein-nucleic recognition.

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